hydrogen atom: center-of-mass and relative

2-particle problem (electron & proton)

$$\left[-\frac{\hbar^2}{2m_e}\Delta_e - \frac{\hbar^2}{2m_p}\Delta_p + V(|\vec{r}_e - \vec{r}_p|)\right]\Psi(\vec{r}_e, \vec{r}_p) = E\,\Psi(\vec{r}_e, \vec{r}_p)$$

separation in center-of-mass and relative coordinates

$$\vec{R} = \frac{m_e\vec{r}_e + m_p\vec{r}_p}{m_e + m_p} \qquad \vec{r} = \vec{r}_e - \vec{r}_p$$

$$M = m_e + m_p \qquad \mu = \frac{m_e m_p}{m_e + m_p}$$

$$-\frac{\hbar^2}{2M}\Delta_R S(\vec{R}) = E_{\mathrm{CM}} S(\vec{R}) \qquad \left[-\frac{\hbar^2}{2\mu}\Delta_r + V(|\vec{r}|)\right]\psi(\vec{r}) = E_{\mathrm{H}}\psi(\vec{r})$$

$$\Psi(\vec{r}_e, \vec{r}_p) = S(\vec{R})\,\psi(\vec{r}) \quad \text{and} \quad E = E_{\mathrm{CM}} + E_H$$

hydrogen atom: spherical separation

relative motion

$$\left[-\frac{\hbar^2}{2\mu}\Delta_r + V(|\vec{r}\,|)\right]\psi(\vec{r}) = E_{\mathrm{H}}\psi(\vec{r})$$

spherical symmetry

$$\psi(\vec{r}) = \frac{u(r)}{r} Y_{l,m}(\theta, \phi)$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right) u(r) = E_H\, u(r)$$

dimensionless units: $\rho = \kappa r$ with $\kappa^2 = 2m|E|/\hbar^2$ and $\rho_0 = 2me^2 / (4\pi\varepsilon_0 \hbar^2 \kappa)$

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1\right) u(\rho) = 0$$

hydrogen atom: radial solution

ansatz (solve asymptotics)

$$u(\rho) = \rho^{l+1}\, w(\rho)\, e^{-\rho}$$

differential equation for *L(s)*:

$$\rho \frac{d^2 w}{d\rho^2} + 2(l + 1 - \rho)\frac{dw}{d\rho} + (\rho_0 - 2(l+1))w = 0$$

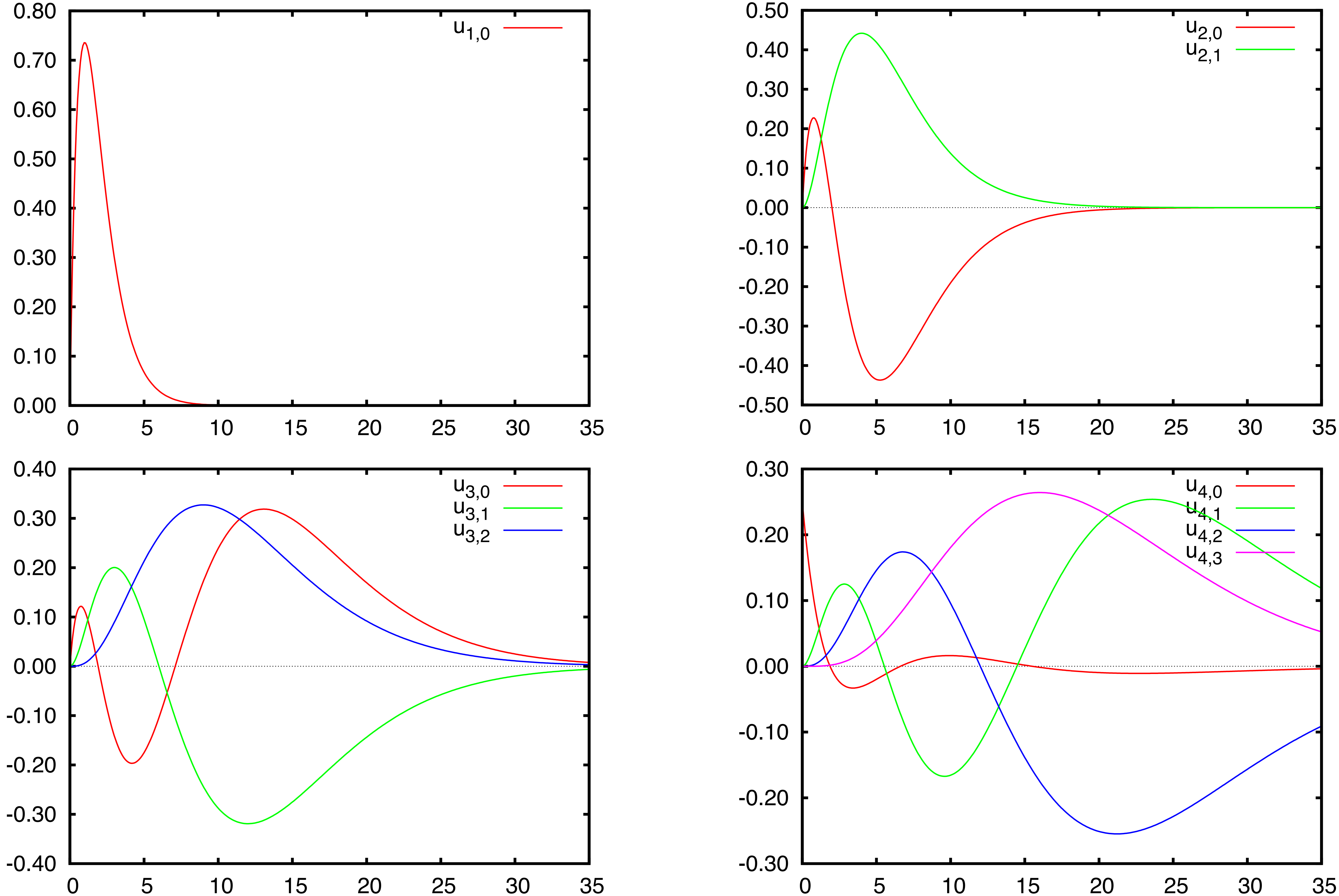
ansatz: power series $$w(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$

recursion for coefficients $$a_{k+1} = -\frac{2(k+l+1) - \rho_0}{(k+1)(k+2l+2)}\, a_k$$

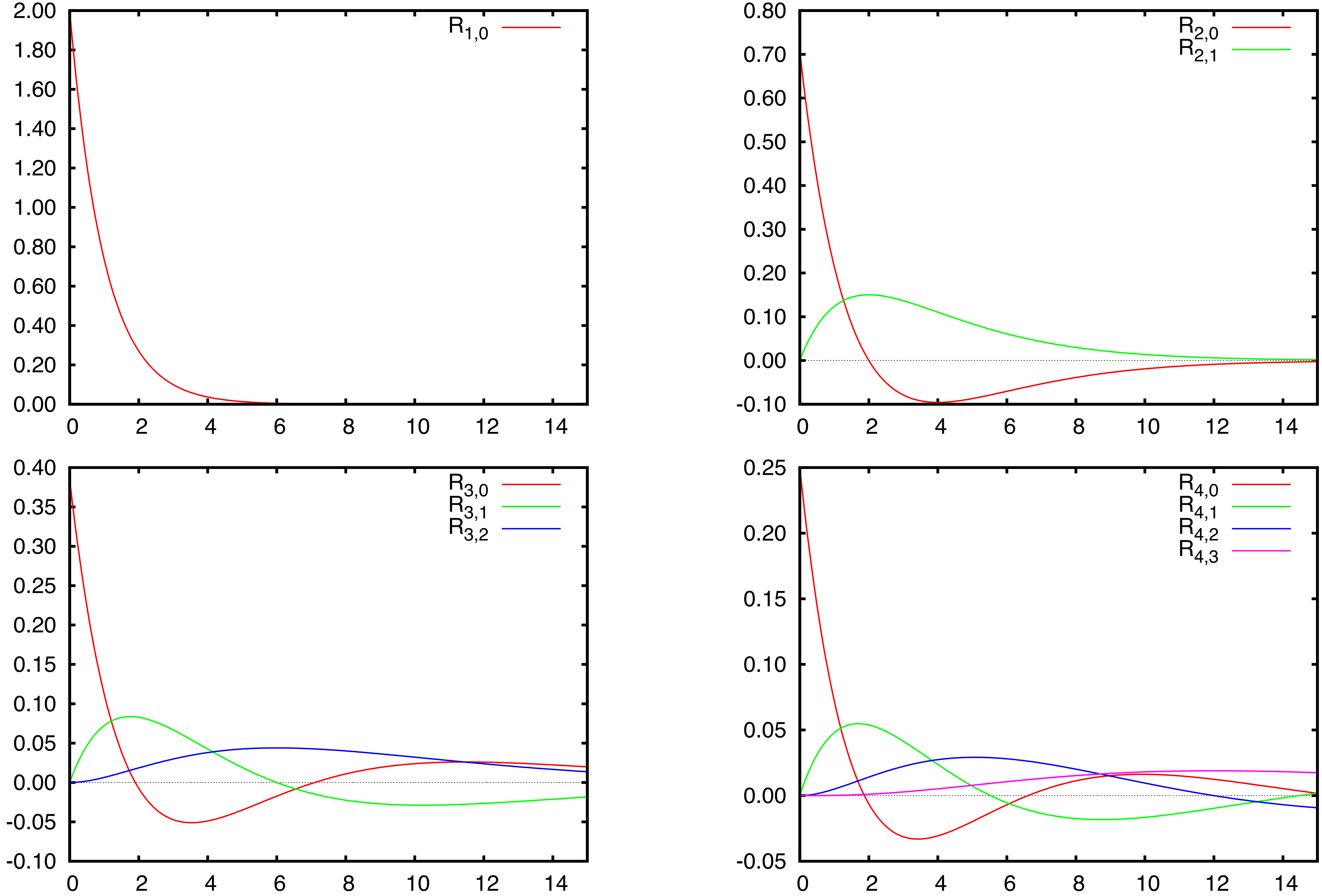
normalizability: recurrence must terminate at some finite *k*

$$n \geq l + 1$$

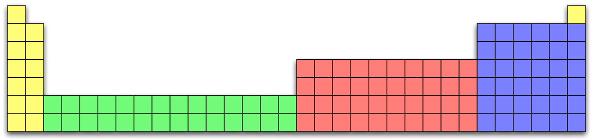
radial functions $u_{nl}(r) = r\,R_{nl}(r)$

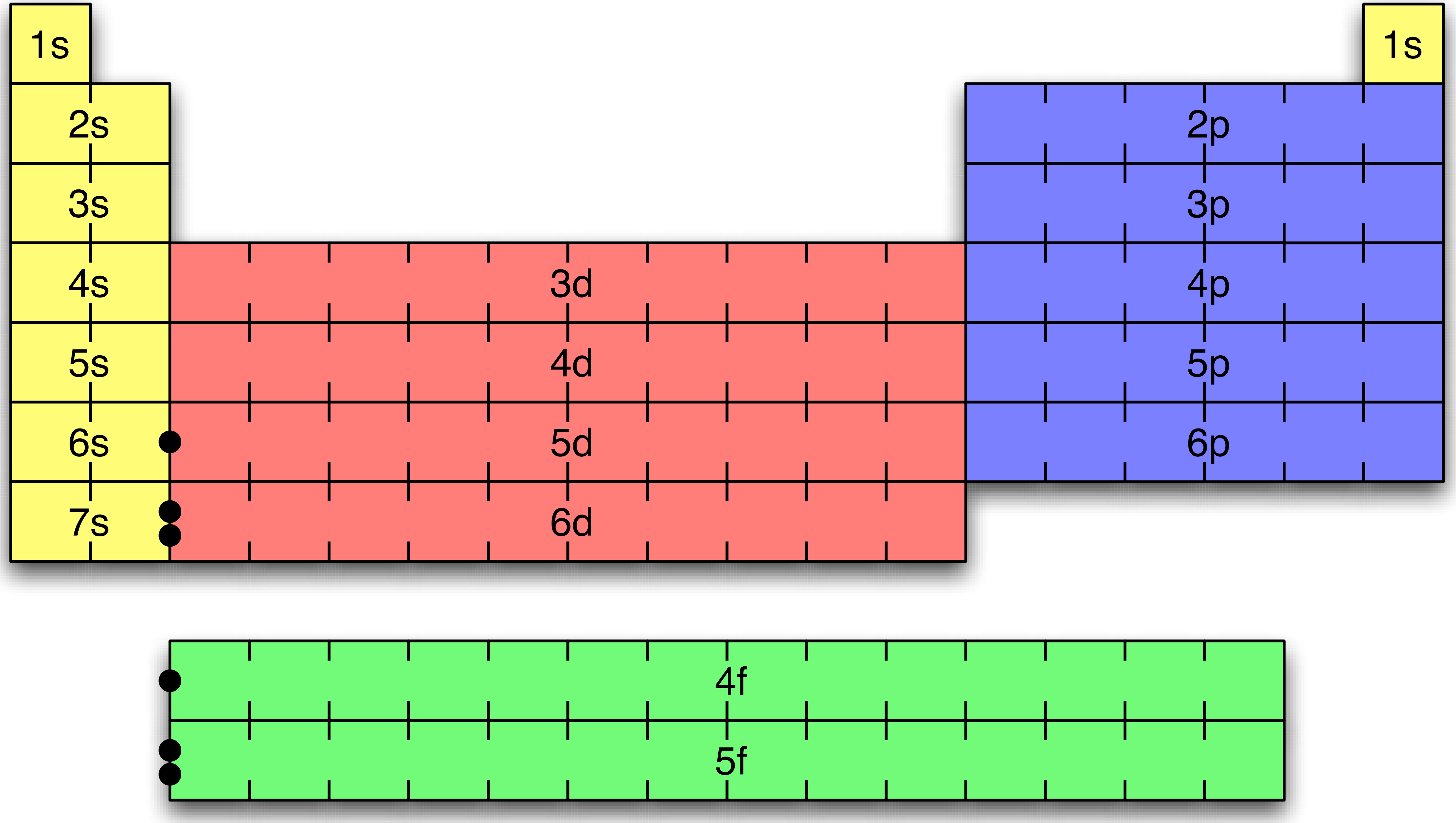


radial functions $R_{nl}(r)$

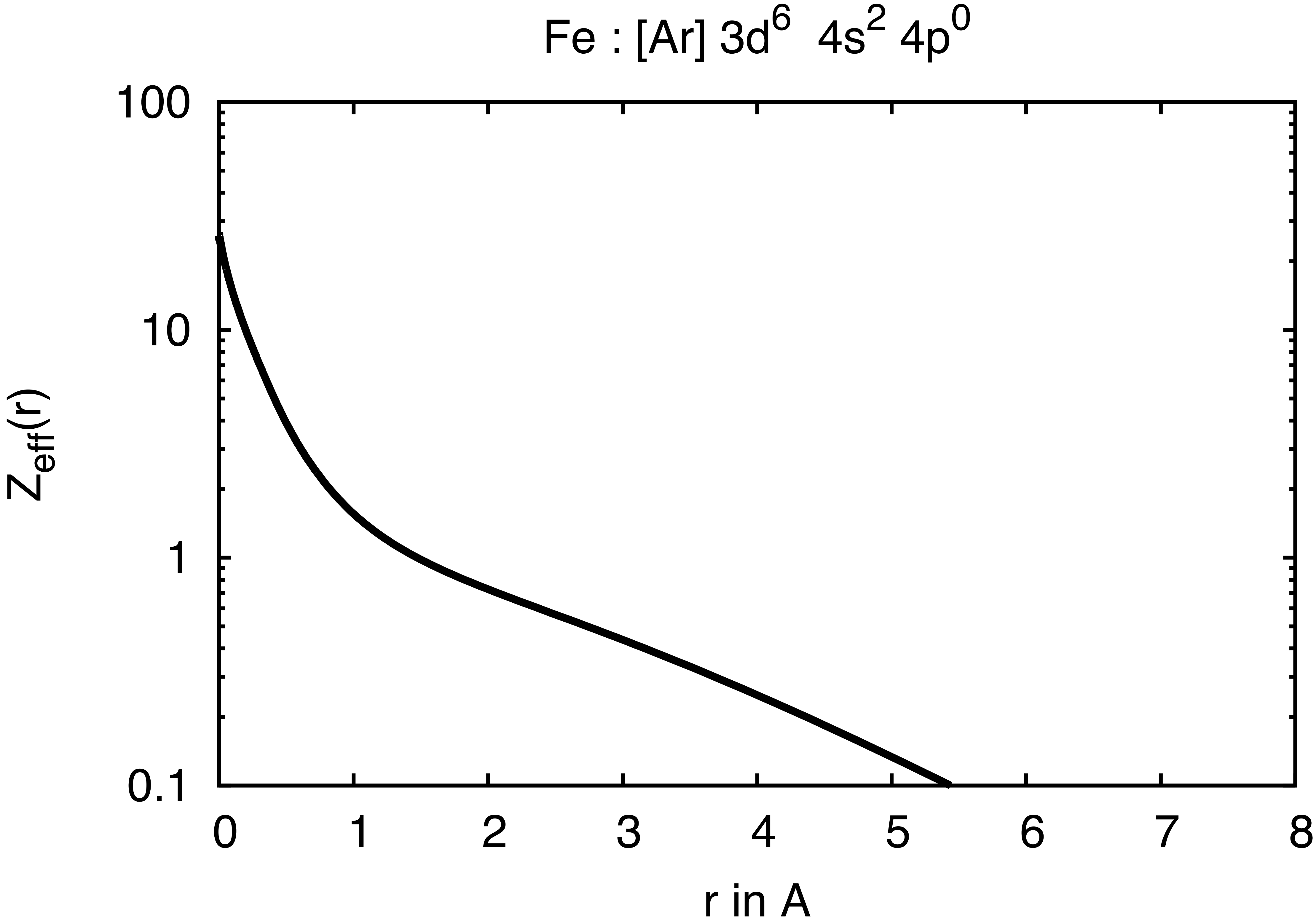


periodic table





atom in spherical mean-field approximation



Atom- und Hybrid-Orbitale